Artificial neural networks for modeling the transfer function between marine reflectance and phytoplankton pigment concentration

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Abstract

A neural network methodology is developed to estimate near-surface phytoplankton pigment concentration of Case I waters from spectral marine reflectance measurements (ocean color) at the SeaWiFS visible wavelengths. The advantages of neural network approximation, i.e., association of non-linear complexity, smoothness, and reduced sensitivity to noise are demonstrated. When applied to in situ CalCOFI data, the neural network algorithm performs better than reflectance ratio algorithms. Relative r.m.s. errors on pigment concentration are reduced from 61 and 62% to 38%, and absolute r.m.s. errors from 4.43 and 3.52 mg m^{-3} to 0.83 mg m^{-3}. When applied to SeaWiFS derived imagery, there is statistical evidence that the neural network algorithm filters residual atmospheric correction errors more efficiently than the standard SeaWiFS bio-optical algorithm.

Keywords

Ocean Color, Neural Networks, Noise Filtering, Phytoplankton, Remote Sensing.

1. Introduction

Quantitative assessment of oceanic primary production and its role in the global carbon cycle is a critical environmental and scientific issue [JGOFS, 1987; Abbott et al., 1994; Falkowski, 1994; Sarmiento and Bender, 1994]. Knowledge of primary production is necessary to calculate new production, derive the effect of biological processes on the partial pressure of carbon dioxide (CO_2), and, therefore, better understand how phytoplankton carbon fixation affects the net CO_2 flux accross the air-sea interface [Behrenfeld et al., 1998]. Primary production depends on light availability and other environmental factors (temperature, nutrients), and on the amount of phytoplankton present for photosynthesis [Morel, 1991]. The amount of phytoplankton and their optical properties (absorption, scattering) affect the spectral diffuse reflectance of the ocean, defined as the ratio of upwelling to downwelling irradiance at a given depth. Since phytoplankton pigments generally absorb more in the blue than in the green, the greener the water, the more phytoplankton [Clarke et al., 1970]. Thus by measuring ocean color, meaning the spectral reflectance at zero depth, $R_w(\lambda)$, one can obtain estimates of phytoplankton pigment concentration, one of the key variables affecting primary production.

A variety of optical transfer functions (bio-optical models) have been proposed to quantify the influence of chlorophyll pigments on spectral reflectance. The bio-optical relationships are generally established by analyzing concomitant reflectances and pigment data. They are non-linear, making inversion difficult for accurate retrieval of pigment concentration. In remote sensing, the most popular algorithms to estimate phytoplankton pigment concentration use simple ratios of reflectances in the blue and green or combinations of ratios [Gordon et al., 1983; Aiken et al., 1995; O'Reilly et al., 1998]. Standard algorithms are based on the ratio of reflectances at 443 and 555 nm, $R_w(443)/R_w(555)$, or 490 and 555 nm, $R_w(490)/R_w(555)$. In some algorithms, empirical laws describing spectral absorption and scattering properties, obtained from the data, are used in semi-analytical reflectance models [e.g., Garver and Siegel, 1997; Carder et al., 1999]; in other algorithms, least mean square fit regressions between measured reflectances and pigment concentration are obtained directly. Recent algorithms compute the logarithm of the pigment concentration, C, from the logarithm of the reflectance ratio using a third order polynomial fit [André and Morel, 1991; O'Reilly et al., 1998].

Blue-green ratios, when applied to satellite-derived marine reflectances, are affected by atmospheric correction errors. It is difficult to achieve accurate atmospheric corrections of the ocean reflectance since typically 80-90% of the signal measured at satellite altitude originates from the atmosphere [Viollier et al., 1980]. Typical errors of 5-10% on the reflectance in the blue are expected with current atmospheric correction schemes, but they may be much larger in the presence of dust or pollution-type aerosols [Gordon and Wang, 1994; Gordon, 1997]. Even though atmospheric correction errors are correlated spectrally, they may not cancel in a ratio, yielding significant, even unacceptable errors on phytoplankton pigment retrievals. Estimates obtained with the Coastal Zone Color Scanner (CZCS) had errors of about 40-50% at low pigment concentrations [Gordon et al., 1980; Gordon, 1983], but part of these errors might be due to variability in phytoplankton type.

As shown in Thiria et al. [1993], Neural Networks (NN's) are good candidates for modeling inverse functions. They have been used in a number of geophysical applications, but it is only recently that attempts have been made to retrieve ocean composition variables with the help of NN's [Schiller and Doerffer, 1998; Keiner and Brown, 1999]. In the present study, we propose a particular class of NN's, called Multi-Layered Perceptrons (MLP's), to compute phytoplankton pigment concentration (chlorophyll-a plus phaeophytin) from satellite-derived marine reflectances. We perform a formal analysis of the capability of NN's to filter noise, thus we focus mainly on methodology. To calibrate our models, we used simulated datasets which take into account instrumental noise, environmental variance and residual atmospheric correction errors. This procedure allowed us to verify the importance of the presence and nature of simulated noise when calibrating the NN's, since we showed that taking into account noise is necessary to extract the inherent information of the geophysical signal and obtain an operational function. We choose a particular ocean color radiometer, the Sea-viewing Wide Field-of-View Sensor (SeaWiFS) onboard the SeaStar satellite, which measures reflected sunlight in spectral bands centered at 412, 443, 490, 510, and 555 nm [Hooker et al., 1992], but the methodology is applicable to other ocean color sensors.

First, leaving aside the problem of atmospheric correction, we evaluate a neural model trained on simulated data containing typical instrumental noise, including environmental variance. We discuss the quality of the direct simulation and neural inversion. We also compare the performance of the NN's educated using the five spectral reflectances with that of the polynomial fits of the classic ratios, $R_w(443)/R_w(555)$ and $R_w(490)/R_w(555)$ (referred to as RR443 and RR490). We examin the differences between these two families of function approximators and the contribution of additional spectral bands.

Second, we consider the case of data contaminated by residual atmospheric correction errors, in order to demonstrate the potential of the NN's for inverting satellite-derived marine reflectances. We apply NN's educated with simulated marine reflectances containing such errors to actual SeaWiFS imagery.

2. Simulated Datasets

Neural networks provide a family of functions that can approximate a wide range of non-linear continuous functions [Thiria et al., 1993; Bishop, 1995]. In Section 3 we will justify and discuss the type of network selected for the study. The ability of NN's to model noise [Bishop,1995] can be exploited, in certain conditions, to filter measurement noise during a model calibration, which is a potentially powerful advantage when dealing with real data. Since it is difficult to gather sufficient data (pairs of marine reflectance and pigment concentration) to educate NN's properly, we decided to use simulated datasets. Our objective is to assess not only the quality of the NN's, but also the importance of adding modeled geophysical noise when only simulated data are available. By contrasting results obtained using clean (i.e. non-noisy) and noisy data, we expect to gain information on the applicability of the theoretical model to real observations. We only consider Case I waters, i.e. waters for which optical properties depend on phytoplankton pigments and their co-varying degradation product, since these waters constitute more than 90% of the world ocean [Morel, 1988].

We simulated spectral marine reflectance, R_w, defined as the ratio of upwelled and downwelled irradiance just below the surface, as a function of phytoplankton pigment concentration, C (chlorophyll-a + phaeophytin), using the bio-optical model of Morel, [1988]. We varied C from 0.03 to 30 mg m^{-3}, the domain of validity of the model. The simulations were made for the SeaWiFS spectral bands centered at wavelengths of 412, 443, 490, 510, and 555 nm (λ_i, with i=1, 2, ..., 5, respectively). Marine reflectance in these spectral bands is differentially sensitive to C. The model of Morel [1988] incorporates average bio-optical parameters determined by regression analysis of in-situ measurements. Absorption and scattering coefficients, on the other hand, vary with the type of phytoplankton population (natural assemblages) [Mitchell and Kiefer, 1988; Mitchell and Holm-Hansen, 1991; Bricaud et al., 1995; Garver and Siegel, 1997]. In the simulations, however, we did not take into account variability due to phytoplankton type. The simulated marine reflectances, therefore, depend only on C. We used new values for the absorption coefficient of optically pure sea water [Pope, 1993; Pope and Fry, 1997]. Consequently, we adjusted Morel's [1988] diffuse attenuation coefficient for phytoplankton, since this coefficient was computed by subtracting the contribution of pure oceanic waters based on previous estimates.

Three types of data were generated; they are summarized in Table 1. The first type of data, hereafter referred to as Type 1 data, was obtained using Morel's [1988] model modified as indicated above. No noise was introduced to the simulated reflectances, nor to the pigment concentrations. These non-noisy data are used to demonstrate the ability of neural networks to model a complex bio-optical function; they also serve as a reference in the study of the effects of noise on the performance of the neural networks. The second type of data, hereafter referred to as Type 2 data, was obtained by adding the same Gaussian noise $\mathcal{N}(0, 0.1)$, Δ_{rad}, to the Type 1 reflectances. This noise, correlated spectrally, is assumed to be typical of under-water radiometers of the MER class (see, e.g. Mueller and Austin, 1995), used to collect the in-situ data analysed in section 4. Spectral correlation is expected since environmental errors (due to ship shadow, clouds, surface extrapolation, surface waves) dominate, and they affect all the spectral bands in a similar way. Furthermore, uncertainties in the radiometric calibration (intensity of the calibration lamps) are likely to have the same sign at all wavelengths. We are aware that the selection of Δ_{rad} is somewhat arbitrary, but spectrally correlated noise is more realistic than uncorrelated random noise in all the spectral bands. The third type of data, hereafter referred to as Type 3 data, includes simulated SeaWiFS-derived reflectances. These reflectances were obtained by adding a three-component noise, Δ_{atm}, to the Type 1 reflectances. This noise is due to (1) radiometric performance, (2) imperfect atmospheric correction, and (3) passage from bidirectional reflectance just above the surface (the SeaWiFS product after atmospheric correction) to irradiance reflectance just below the surface, the variable related to C in Morel's [1988] model. We assumed, when computing Δ_{atm}, that the atmospheric correction is performed according to Gordon and Wang, [1994], i. e. by obtaining aerosol information in the near-infrared where the ocean is "black" and extrapolating the information to the visible. We give a detailed description of Δ_{atm} in the Appendix.

In order to have staticsally significant results, we dealt with a large amount of data. The inverse models (NN, RR443 and RR490) were calibrated using the same 5000 vectors of simulated pairs of $\{\mathrm{C}^k, \mathrm{R}^k_{wn}(\lambda_i)$, i=1...5$\}$ (n=1, 2, or 3) and tested with independent test sets of 10,000 simulated vectors with the same characteristics called Test-1, Test-2 and Test-3. We obtained, consequently, three different neural inverse models and six different classical inverse models denoted as described in Table 1. We characterized model performance correlation coefficient, r^2, RMS error and relative RMS error. The last two indices are defined as:

$$RMS = \sqrt{\frac{1}{N_{test}} \sum_{k=1}^{N_{test}} \left[\mathrm{C}^k - F(\vec{\mathrm{R}}^k_w, \mathcal{W})\right]^2}$$

$$rel.RMS = \sqrt{\frac{1}{N_{test}} \sum_{k=1}^{N_{test}} \left[\frac{\mathrm{C}^k - F(\vec{\mathrm{R}}^k_w, \mathcal{W})}{\mathrm{C}^k}\right]^2}$$

where N_{test} is the number of patterns in the test set and $F(\vec{\mathrm{R}}^k_w, \mathcal{W})$ refers to the inverse model.

3. Multi-Layered Perceptrons

In this section we provide a basic description of the Multi-Layered Perceptrons (MLP's), and of the properties they offer for non-linear regression. Then we discuss the numerical methodology employed to optimize the parameters of such non-linear models.

3.1. Definitions and properties

MLP's have been used by Thiria et al. [1993] to model complex inverse functions. We recall here their major properties. A neuron is an elementary transfer function which calculates an output s when an input $\mathcal{A}$ is applied:

$$s = f(\mathcal{A}) \tag{1}$$

where f is called the transition function and is usually non-linear. A neural network is formed by interconnected neurons, each neuron receiving and sending signals only to the neurons to which it is connected. MLP is a particular class of neural networks in which neurons are organized in several layers. The state s_j of a neuron j is computed by $s_j = f(\mathcal{A}_j)$, where $\mathcal{A}_j$ is the total information received from the other neurons s_h computed as a weighted sum $\mathcal{A}_j = \sum_h w_{jh} s_h$. The transition function f can be linear, i.e. $f(u) = u$ for the exit layer, or a sigmoid with

$$f(u) = a\frac{\exp(\alpha u) - 1}{\exp(\alpha u) + 1} \tag{2}$$

We dealt with $a = 1.7159$ and $\alpha = 1.3333$ so that f was quasi-linear in the range $[-1 : 1]$, $f(-1) = -1$ and $f(1) = 1$. The w_{jh} are the connection weights from h to j; they are real numbers parameterizing the influence of the connected neurons. The weight matrix $\mathcal{W} = [w_{jh}]$ defines the MLP specifity.

Theorical considerations show that MLP's are universal function approximators [Bishop, 1995]. In our case, defining an architecture, i.e. deciding the number of neurons and the way they are connected, represents choosing a function's family in which we seek the best function allowing us to invert spectral in-waters reflectances $\mathrm{R}_w(\lambda_i)$ into pigment concentration C. We then solve a regression problem since we have to optimize MLP weights to obtain the best estimated model. The w_{jh} values are computed by a calibration process in which the input and output of the MLP are well-defined data sets, and the w_{jh} values are the control variables. This learning process is based on a cost function minimization (Section 3.3). When the calibration is done, MLP inverse model does algebric operations only, leading to fast computation.

3.2. Architecture

Given the flexibility of MLP's, we chose to take into account all the available information, so we related the five Sea-WiFS spectral reflectances to the pigment concentration, C. Our problem was then to determine a multidimensional real function which approximates the transfer function between the vector $\{\mathrm{R}_w(\lambda_i), i = 1..5\}$ and the scalar C. We determined the best architecture using a constructing methodology which makes intensive use of cross validation [Bishop, 1995]. For inverting Morel's [1988] model (type 1 data, *cf* §2), we obtained a completely connected MLP with five inputs (the five spectral in-waters reflectances), two hidden layers of six and four sigmoid neurons, and one linear output which gives the concentration C. This network, denoted NN-1 hereafter, has 69 parameters to be adjusted including bias parameters (see Fig. 1). We used the same architecture to invert the noisy reflectances (type 2 and 3 data) and denoted NN-2 and NN-3 the MLP's trained on type 2 data and type 3 data, respectively (see Table 1).

3.3. Parameter estimation

For the learning process, we chose to minimize the mean quadratic error computed on a learning ensemble of N observations, thus to use a least-square method. Learning consists here of minimizing an empirical cost $\mathcal{J}$ defined as:

$$\mathcal{J}(\mathcal{W}) = \sum_{k=1}^{N}\left[\mathrm{C}^k - F(\vec{\mathrm{R}}_w^k, \mathcal{W})\right]^2 \tag{3}$$

where C^k is the desired concentration of the observation k, and $F(\vec{\mathrm{R}}_w^k, \mathcal{W})$, the corresponding concentration computed by the neural model, which is a function of the reflectance vector $\vec{\mathrm{R}}_w^k$ and internal parameters set by the weight matrix $\mathcal{W}$. A necessary condition to minimize $\mathcal{J}$ is to find the neural weight matrix $\mathcal{W}^*$ so that:

$$\nabla\mathcal{J}(\mathcal{W})\,|_{\mathcal{W}=\mathcal{W}^*} = \left\{\frac{\partial\mathcal{J}(\mathcal{W})}{\partial w_{hj}}\right\}_{\forall h, \forall j} |_{\mathcal{W}=\mathcal{W}^*} = 0 \tag{4}$$

To approach the minimum of this multidimensional cost function, we used a gradient technique which is an iterative optimization method, adapted to multi-layered perceptrons by gradient backpropagation [Bishop, 1995]. A serie of cross validation tests allowed us to control the quality of the minimum estimation and of the generalization. Theory shows that, if the architecture of the MLP is well-chosen, the minimization of $\mathcal{J}(\mathcal{W})$ is well achieved, and the observation set is consistent with the true field of variables, the MLP then gives an accurate approximation of the mean field of the variable C [Bishop, 1995]. More precisely:

$$F(\vec{\mathrm{R}_w}, \mathcal{W}) \approx E[\mathrm{C}/\vec{\mathrm{R}_w}] \quad (5)$$

where $E[\mathrm{C}/\vec{\mathrm{R}_w}]$ is the conditional average of the concentration C for each point $\vec{\mathrm{R}_w}$. This allowed us to fit the desired non-linear transfer function using noisy data. The three order polynomial fits RR443 and RR490 were also calibrated using the least-square method, so that the performance of classical approaches and NN's would be comparable.

4. Performance of the NN-1 and NN-2 models

4.1. Results using synthetic data

In this section we discuss the performance we obtained by testing the NN-1 and NN-2 models after training on the two test sets of type 1 and type 2 data. In the following, the retrieval of pigment concentration by NN's inverse models is displayed using scatter plots. Fig. 2a demonstrates the high fidelity of neural inversion NN-1 on type 1 data, and so the ability of NN's to invert complex mathematical function. Fig. 2b shows the NN-2 results on noisy type 2 data. NN-1 and NN-2 exhibit a similar behaviour showing the ability of NN-methodology to take into account the effects of noise. Further investigations using cross tests allow us to understand the properties of the two NN's inverse models. We first test NN-2 on type 1 data (i.e. data with no noise). The scatter plot of Fig. 3a proves that NN-2 is a generalisation of NN-1. On the contrary, NN-1 cannot deal with noisy data: the scatter plot of NN-1 when tested with noisy data shows a degradation of the performance (Fig. 3b). Table 2 gives the statistical parameters obtained for the four different experiments.

To make a comparison, we also evaluated the performance of the classical inverse models RR443-1 and RR490-1 calibrated on type 1 data and of RR443-2 and RR490-2 calibrated on type 2 data. The inversion of type 1 and type 2 data is correct for both NN's and polynomial fits. Since the simulated noise Δ_{rad} is the same for all wavelengths, the effects of such noise disappears when making a ratio of the spectral reflectances, and so, the results of polynomials fits on type 1 and type 2 data are similar. While the NN-1 (or NN-2) inversion is quasi-perfect from small to large values of concentration, the precision given by the polynomial fits decreases (in a oscillating way) with increasing concentration, from 2% to 10% for RR490-1 (or RR490-2) and 5% to 14% for RR443-1 (or RR443-2), but the performance remains reasonable.

4.2. Results using in situ data

In the previous section we showed that NN's inverse models are able to deal with synthetic data and to take into account realistic, but simulated, underwater radiometer errors (Δ_{rad}). In order to check this result on real data, we performed additional experiments. The performance of neural and classical inverse models calibrated using simulated type 1 and type 2 data were tested with in situ measurements, collected during several California Cooperative Oceanic Fisheries Investigation (CalCOFI) campaigns between August 1993 and October 1996.

The in situ measurements were obtained by an integrated underwater profiling system which was able to collect optical data and to characterize the water column. This system included an underwater MER-2040 radiometer (Biospherical Instruments Inc., S/N 8738) which acquired depth profiles of downwelling spectral irradiance, E_d, and upwelling radiance, L_u, at the nominal wavelengths of our interest: 412, 443, 490, 510 and 555 nm. In order to create our test-set, values for L_u and E_d just below the surface were obtained by extrapolation to zero depth [Mitchell and Kahru, 1998]. We transformed the ratio $R_{rs}=L_u/E_d$ into $R_w=E_u/E_d$ (where E_u is the upwelling irradiance) using the following relation:

$$R_w = \mathcal{Q} \cdot R_{rs} \tag{6}$$

where the $\mathcal{Q}$ factor is taken according to Morel and Gentili [1993, 1996]. Water sampling during CalCOFI cruises was done with a CTD-rosette system separate from the MER profiler. The chlorophyll-a and phaeopigment concentrations were determined by the fluorometric method [Holm-Hansen et al., 1965; Venrick and Hayward, 1984].

The MER 2040 unit and associated underwater instruments were deployed using the ship's stern A-frame on each station in accordance with SeaWiFS bio-optical protocols [Mueller and Austin, 1995]. Processing of the CalCOFI bio-optical profiles is described in detail in Mitchell and Kahru, [1998]. The radiance L_u measured by an instrument of a finite size is affected by the instrument's own shadow [Gordon and Ding, 1992]. The self-shading correction scheme recommended by Mueller and Austin, [1995] has been implemented in the analysis since 1997 [Mitchell and Kahru, 1998]. For the data we used here the instrument self-shading was ignored. The median error resulting in underestimating L_u for the SeaWiFS bands of the CalCOFI data was 1-2% while the maximum error was about 20% for high pigment water. Moreover large values of pigment concentration (more than 10 mg m^{-3}) were obtained in coastal waters which were probably Case II waters. We consequently chose not to test high pigment data.

Comparing the performance of the two different neural models (Fig. 4), we can see that the neural network NN-2, which was trained on noisy simulated data, is able to invert real measurements (Fig. 4b), not perfectly but much better than NN-1, which is simply the inverse of Morel's [1988] model (Fig. 4a). We can also compare the performance of NN's and bands ratios tested with CalCOFI data (Fig. 5). The results of RR443-1 and RR490-1 are exactly the same as RR443-2 and RR490-2 because of our choice of Δ_{rad} (see Section 2), so we present only the performance of type 1 band ratio. The results of the polynomial fits (type 1 or 2) are comparable to those of NN-2, except at low and high C values where band ratios have larger errors. The biases in Figs. 4b and 5, however, are largely caused by the imperfect fit of the Morel's [1988] model to the CalCOFI observations. Table 3 gives the statistical parameters obtained for the four experiments. By plotting the relative RMS error as a function of C for NN-2 and polynomials fits (Fig. 6), we can see the advantage of using a NN trained on noisy data, for this approach gives a consistent inverse model with little dependence on concentation range.

Thus NN's inverse models appear to give improved performance when dealing with in situ data. Retrieval of pigment concentration using satellite ocean color measurements is even more complex due to atmospheric correction errors. In the next section we extend our results to satellite-derived reflectances.

5. Effect of residual atmospheric correction noise

We explored, using simulated data only (types 1 and 3), the capability of NN's to minimize the problem of residual atmospheric correction errors, and we examined the results by comparing the performance of neural models to that of the third order polynomial fit usually employed to invert ocean color. The Appendix describes our approach to simulate atmospheric correction noise for our modeled data set.

Fig. 7 shows the performance of NN-3, the neural inverse model trained on atmospherically noisy data (type 3). The curve is scattered by the simulated uncertainty of the measurements, but there is no bias. As in Section 4, we performed cross tests with results comparable to those provided by NN-1 and NN-2. We verified that NN-3 is a generalisation of NN-1 by testing NN-3 on type 1 data (see Fig. 8a), and as expected, NN-1 was inadequate for noisy type 3 data, as depicted by the large scatter of Fig. 8b. The performance statistics are summarized in Table 4. Clearly, the relative RMS error of 5.48% achieved by NN-3 when dealing with Test-3 data indicates a good fit of the data.

We ran comparison on Test-3 data using the polynomial fits based on band ratios RR443-3 and RR490-3 calibrated with type 3 data. The scatter plots for the two methods given in Fig. 9 are to be compared with those of Fig. 7. The fit is less dependent on pigment concentration for the NN-3 inverse model than for RR443-3 and RR490-3. The band ratio methods are least satisfactory at small and high pigment concentrations. The performance statistics of NN-3, RR443-3, and RR490-3 are summarized in Table 5. Using band ratios instead of NN, the relative RMS error is degraded by a factor of 4-5.

In Fig. 10 the relative RMS error of the three inverse models is displayed for different ranges of C. The polynomial fits perform poorly with simulated atmospheric correction errors. For small pigment concentrations, relative errors may reach 30 and 50%. It appears difficult, therefore, to reach SeaWiFS mission goal of 35% inaccuracy in C using band ratio methods applied to satellite-derived reflectances. On the other hand, the NN gives relative errors around 3% below 1 mg m^{-3} and 10% above 10 mg m^{-3}. This dramatic improvement in relative error makes the NN's approach particulary adapted to satellite imagery.

6. Application to SeaWiFS imagery

To check the sensitivity of the NN's approach to atmospheric correction errors, we applied NN-3 to SeaWiFS Global Area Coverage (GAC) imagery (4 km resolution) acquired on March 11, 1998 off the California coast. The imagery was provided by the Goddard Distribution Active Archive Center. The diffuse marine reflectance just below the surface, R_w, obtained after atmospheric correction (performed by the SeaWiFS project according to Gordon and Wang, 1994), is displayed in Fig. 11 for the five ocean color bands of the instrument. Land, clouds, and flagged pixels are shown in black, and negative values in yellow. The images exhibit a lot of negative values at 412 and 443 nm, especially in the Gulf of California and along the northern California coast, and fewer negative values at the other wavelengths, suggesting imperfect atmospheric correction. In the northern part of the Gulf of California, high reflectance values (> 0.1) at 490, 510, and 555 nm reveal the presence of Case II waters.

The pigment concentrations obtained by the SeaWiFS project's bio-optical algorithm and by NN-3 are displayed in Fig. 12, as well as the difference between the two types of concentrations. In the SeaWiFS project's algorithm, the pigment sum is derived from the chlorophyll-a estimated using the OC2 cubic polynomial function (see O'Reilly et al., 1998). The OC2 algorithm only makes use of the R_{rs} ratio for 490 and 555 nm. Pigment concentration in the standard SeaWiFS product is computed even when reflectances at shorter wavelengths are negative. Using NN-3, however, pigment concentration was only estimated when marine reflectance was positive in all the ocean color bands. NN-3 generally gives higher values than OC2, except in the northern part of the Gulf of California where, on the contrary, the NN-3 values are much lower than OC2's. In this region of Case II waters, NN-3 interprets the high reflectance values in the blue as those of low-pigment waters (remember that NN-3 was only educated with marine reflectances simulated for Case-I waters). Spatial gradients in coastal regions appear sharper in the NN-3 pigment concentration image. In the open ocean where pigment concentration is low, small-scale spatial variability is reduced.

To investigate in more detail the small-scale spatial variability in the satellite-derived pigment concentration images, we examined the pigment concentration along a transect in oligotrophic waters in the western region of the image (see Fig. 12 for location of the transect). In Fig. 13, OC2 and NN-3 pigment concentrations are plotted as a function of sample number along the transect. The OC2 values are generally lower than the NN-3 values, and reach a minimum value of about 0.015 mg m^{-3}. These extremely low values are the arbitrary lower limit allowed by the standard SeaWiFS processing. The minimum value obtained using NN-3 is about 0.05 mg.m^{-3}, which is more realistic for the studied region. Interestingly, the pixel-to-pixel changes are much larger for OC2 than NN-3. In this region of the open ocean, low in pigment concentration, pixel-to-pixel changes are not likely to be due to biological variability, but rather to marine reflectance errors, coming essentially from imperfect atmospheric correction. NN-3 thus appears to be less sensitive to residual atmospheric correction noise than OC2.

We further evaluated this result by statistical analysis of pigment concentration differences as a function of sample distance. We computed, for the oligotrophic region identified by a green rectangle in Fig. 12, an average one-dimensional structure function, SF, defined as:

$$SF(d) = \frac{1}{N_l(N_k - d)} \left\{ \Sigma_i \left[\Sigma_j (C_{i,j} - C_{i,j+d})^2 \right] \right\} \tag{7}$$

where d is the sample distance (in number of pixels), N_l and N_k are the numbers of lines and samples in the selected area, respectively, and $C_{i,j}$ is the pigment concentration of pixel characterized by line i and sample j. The summation over i is from 1 to N_l, and that over k from 1 to $N_k - d$. The function $SF(d)$ is displayed in Fig. 14 for both NN-3 and OC2. Despite the lower C values obtained with OC2 (see Fig. 13), the SF values are higher with OC2, but they increase more smoothly with increasing sample distance. If there were no noise in the pigment concentration field, SF would go to zero when d goes to zero. This is not the case, however, especially for OC2. Using this algorithm, spatial structures of less than 0.001 (mg $m^{-3})^2$, or 0.03 mg m^{-3}, cannot be detected. Using NN-3, specifically educated to account for residual atmospheric correction errors, the SF values are much lower at small sample distances, and the barely detectable wavy structure of the OC2 structure function becomes more apparent. Thus there is strong evidence in the satellite imagery that the NN's approach reduces the effect of atmospheric correction errors on C estimates, as predicted theoretically in section 5 (see Fig. 10), and that the atmospheric correction noise generated to educate NN-3 is realistic, at least for low pigment concentrations.

7. Discussion and conclusion

We described a neural network methodology to solve the ocean color inverse problem of phytoplankton pigment concentration retrieval from in-water reflectances (case I waters). We trained several models using three different types of simulated data. The first neural network (NN-1) was the inverse of the bio-optical model of Morel [1988], the second (NN-2) was trained to inverse in situ measurements, and the third (NN-3) to inverse satellite-derived reflectances. To simulate the data corresponding to NN-2 and NN-3, we added to the in-water reflectances calculated by the bio-optical model a Gaussian noise (similar to the measurement errors in the CalCOFI dataset) or typical atmospheric correction errors made during processing of satellite radiometer reflectances (we took the case of SeaWiFS). The performance of each neural model was compared to that of the third order polynomial fit based on band ratio usually employed to retrieve pigment concentration. These experiments allowed us to understand the conditions where NN's improved the retrieval of pigment concentration and to show the importance of simulating the appropriate noise when the data sets used to calibrate the NN's are modeled.

The NN-1 model gives a quasi-perfect inversion of Morel's [1988] model (0.14% of relative RMS error), and the polynomial fits give also reasonable results (less than 15% of error). However, there is instability in the precision given by the polynomial fits on the whole range of concentration C, which is probably due to the intrinsic oscillations of the polynomial family. The NN's are by definition very soft function approximators, which proves advantageous for this application.

The NN-2 model effectively minimized the measurement errors (mostly environmental) of the in situ dataset, but the performance statistics were not ideal for several reasons. First the Gaussian noise we added is only an approximation, and second, the bio-optical model of Morel [1988] we used to simulate the basic in-waters reflectances does not include all natural variability (Section 2). Here we can see the limitations of the simulation; better results could be reached if we could model the biological variance more accurately.

NN-2 model is a generalisation of NN-1 for it is able to invert Morel's [1988] model. This quality (see numerical results of Table 2) comes from the properties of the quadratic error minimization: a calibration on noisy data gives the estimation of the conditional average (Section 3.3), which is more or less the true expected function when the simulated noise is Gaussian. On the contrary, the NN-1 model is not able to deal with type 2 data or in situ measurements because NN's are incapable of accurate inversion of noisy data when the noise has not been learned during the training phase.

The performance of the NN-3 model is superior to that of the polynomial fits usually employed to compute pigment concentration: NN-3 gives a 3% precision and the polynomial fits were between 30 and 50% for small concentration values, typical of more than 90% of the oceans. This shows that NN-3 is able to filter atmospheric correction errors using the information given by the five spectral bands of SeaWiFS. This was confirmed by applying the NN-3 model to actual SeaWiFS-derived marine reflectance imagery. The small scale variability observed in the standard SeaWiFS product, most probably due to atmospheric and instrumental noise, was reduced substantially using the NN-3 model.

NN's are complex, stable, and adaptative approximators capable of minimizing the effects of measurement errors if properly trained. If the neural models are trained on simulated data as in the present experiments, the quality of the simulation of the measurement noise is fundamental. Using a model like that of Morel [1988] to simulate in-water reflectances and adding a simple and empirical estimation of measurement errors, allowed us to accomplish an accurate inverse transfer function between in-situ measurements of reflectances and pigment concentration. The results obtained using CalCOFI data, demonstrate that the NN's are able to invert in-situ optical parameters with high fidelity. The formal experiment made only on simulated data allowed us to evaluate NN's performance for satellite reflectances with atmospheric correction errors. With sufficiently large in situ data sets the NN's performance could be improved through training on real rather than simulated data.

Appendix: Noise on satellite-derived marine reflectances

Atmospheric correction of SeaWiFS data is accomplished according to Gordon and Wang [1994] (see also Gordon, 1997). First, the satellite signal is corrected for gaseous absorption, molecular scattering, and surface reflection effects (sun glint, sky reflection, whitecaps). Next, the wavelength dependence of the aerosol scattering is obtained from measurements in the red and near-infrared (spectral bands centered at 765 and 865 nm), where the ocean reflectance is assumed to be zero. The amount of aerosol scattering at 865 nm is also determined. Finally, the aerosol effect at ocean color wavelengths (i.e. in the blue and green) is estimated by extrapolation of the aerosol information obtained at the longer wavelengths. The extrapolation is a major source of error, because the wavelengths of 765 and 865 nm are close together and far from the ocean color wavelengths. Furthermore, because the aerosol signal in the near-infrared is mainly affected by the coarse particle mode of aerosols, it contains little information about the accumulation mode. Yet the accumulation mode has strong scattering effects in the visible.

SeaWiFS data, after correction of atmospheric and surface effects, yield bi-directional marine reflectance, ρ_w, defined as the ratio of upwelled radiance times π and downwelled irradiance just above the surface. The irradiance reflectance, R_w, used in Morel's [1988] bio-optical model, is related to ρ_w by the following equation:

$$R_w(\lambda) = \frac{A}{f/\mathcal{Q}} \cdot \rho_w(\lambda) \quad \text{(A1)}$$

where λ is wavelength, and A is a coefficient approximately equal to 0.2. The factor $f/\mathcal{Q}$ depends on geometry (sun and view angles) among other variables, but remains fairly constant for remote sensing conditions, with an average value of 0.0922 [Morel and Gentili, 1993]. In Eq. A1, the satellite-derived reflectance ρ_w can be expressed as

$$\rho_w(\lambda) = \left[\rho_{sat}(\lambda) - \epsilon(\lambda, \lambda_r)\rho_a(\lambda_r)\right]/t_d(\lambda) \quad \text{(A2)}$$

where ρ_{sat} is the top-of-atmosphere SeaWiFS reflectance corrected for gaseous absorption, molecular scattering, sunglint and whitecap effects, t_d is the diffuse atmospheric transmittance (surface-to-satellite), ρ_a is the aerosol reflectance (includes interaction between surface reflection and scattering), ϵ is the spectral dependence of the aerosol reflectance, and λ_r is a wavelength of reference in the near-infrared (λ_r = 865 nm).

The relative error on $\mathrm{R}_w(\lambda)$ is given by

$$\frac{\Delta \mathrm{R}_w(\lambda)}{\mathrm{R}_w(\lambda)} = \frac{\Delta\rho_w(\lambda)}{\rho_w(\lambda)} + \frac{\Delta(f/\mathcal{Q})(\lambda)}{(f/\mathcal{Q})(\lambda)} \quad \text{(A3)}$$

with

$$\Delta\rho_w(\lambda) = \frac{1}{t_d(\lambda)}[\Delta\rho_{sat}(\lambda) + \rho_a(\lambda_r)\Delta\epsilon(\lambda,\lambda_r) + \epsilon(\lambda,\lambda_r)\Delta\rho_a(\lambda_r)] \quad \text{(A4)}$$

Assuming that

$$\epsilon(\lambda, \lambda_r) = \gamma(\lambda_r/\lambda)^n \quad \text{(A5)}$$

where n is the Angström exponent (characterizes the spectral dependence of the aerosol optical thickness) and γ the ratio of aerosol phase functions at λ and λ_r (approximately equal to 0.9; see Viollier et al., 1980), the last two terms on the right-hand side of Eq. A4 can be written:

$$\begin{aligned} \Delta_1\rho_w(\lambda) &= \frac{1}{t_d(\lambda)}\rho_a(\lambda_r)\Delta\epsilon(\lambda,\lambda_r) \\ &= \frac{1}{t_d(\lambda)}\gamma(\lambda_r/\lambda)^n\rho_a(\lambda_r) \\ &\quad \times \ln(\lambda_r/\lambda)\Delta n \quad \text{(A6)} \\ \Delta_2\rho_w(\lambda) &= \frac{1}{t_d(\lambda)}\epsilon(\lambda,\lambda_r)\Delta\rho_a(\lambda_r) \\ &= \frac{1}{t_d(\lambda)}\gamma(\lambda_r/\lambda)^n\Delta\rho_a(\lambda_r) \quad \text{(A7)} \end{aligned}$$

Conveniently, the error $\Delta_1\rho_w$ at any wavelength λ can be expressed as a function of the error $\Delta_1\rho_w$ at 443 nm (Δn in Eq. A6 disappears). This leads to

$$\Delta_1\rho_w(\lambda) = \frac{\Delta_1\rho_w(443)t_d(443)\ln(865/\lambda)}{(443/\lambda)^n t_d(\lambda)\ln(865/443)} \quad \text{(A8)}$$

Note that no error on t_d is assumed in Eq. A2 and subsequent equations because the effect of aerosols on t_d is small. Typical values of t_d are 0.7-0.8 at blue and green wavelengths [Deschamps et al., 1983]. Since it is the ratio of γ and t_d or of t_d's at two wavelengths that appears in Eqs. A7, and A8, and since γ and t_d's have similar values, the effect of γ and t_d on the errors $\Delta_1\rho_w(\lambda)$ and $\Delta_2\rho_w(\lambda)$ is neglected. According to Gordon and Wang [1994] and Gordon [1997], ρ_w in the blue can be retrieved with a typical accuracy of $\pm 5 - 10\%$ in clear waters. The value of $\pm 5\%$ is used for $\Delta_1\rho_w(443)/\rho_w(443)$. For $\rho_{sat}(\lambda)$ and $\rho_a(\lambda_r)$, uncertainties in the correction of molecular scattering and other effects are neglected, and $\Delta\rho_{sat}(\lambda)$ and $\Delta\rho_a(865)$ are fixed at the SeaWiFS radiometric noise, taken from Table 1 of Gordon [1997]. The factor $f/\mathcal{Q}$ varies by about $\pm 7\%$ around the average value of 0.0922 and increases with sun zenith angle [Morel and Gentili, 1993]. The coefficient A in Eq. A1 is inaccurate to $\pm 3\%$ (see Gordon et al., 1988). Uncertainties in $f/\mathcal{Q}$ and A partly compensate; both uncertainties are correlated spectrally. Therefore, $\Delta(f/\mathcal{Q})/(f/\mathcal{Q})$ is assumed to be $\pm 5\%$ in all the spectral bands.

Thus in the simulations of type 3 reflectance data, a noise $\Delta_{atm} = \Delta \mathrm{R}_w$ (Eqs. A3, A7, A8) is added to R_w. This noise is generated using independent random numbers for $\Delta_1\rho_w(443)$, $\rho_a(865)$, $\Delta\rho_{sat}(\lambda)$, n, and $\Delta(f/\mathcal{Q})$. The Angström exponent is varied between 0 and 2, the range of values generally encountered over the oceans.

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Table 1. Statistical Ensembles for Neural Network Calibration and Notation of the Various Inverse Models.

Ensemble	Description	NN's	Polynomial fits
Type 1	$R_{w1}(\lambda_i)$ = f(C, mg.m^{-3}) from Morel [1988]	NN-1	RR443-1 and RR490-1
Type 2	$R_{w2}(\lambda_i) = R_{w1}(\lambda_i) + \Delta_{rad}$	NN-2	RR443-2 and RR490-2
Type 3	$R_{w3}(\lambda_i) = R_{w1}(\lambda_i) + \Delta_{atm}(\lambda_i)$	NN-3	RR443-3 and RR490-3

Table 2. Performance of NN-1 and NN-2, Tested on Test-1 and Test-2 Ensembles.

	NN-1		NN-2	
Statistical Parameter	Test-1	Test-2	Test-1	Test-2
RMS error (mg.m^{-3})	0.024	2.138	0.014	0.019
rel. RMS error (%)	0.14	59.02	0.10	0.14
coeff. r^2 (%)	99.99	95.81	99.99	99.99

Table 3. Performance of the Various Inverse Models Tested on CalCOFI Data.

Statistical Parameter	NN-1	NN-2	RR443-1	RR490-1
RMS error (mg.m^{-3})	0.81	0.83	4.43	3.52
rel. RMS error (%)	77	38	62	61
coeff. r^2 (%)	76	87	81	93

Table 4. Performance of NN-1 and NN-3, Tested on Test-1 and Test-3 Ensembles.

	NN-1	NN-3	
Statistical Parameter	Test-3	Test-1	Test-3
RMS error ($mg.m^{-3}$)	0.93	0.13	0.73
rel. RMS error (%)	21.90	2.85	5.48
coeff. r^2 (%)	99.13	99.97	99.41

Table 5. Performance of RR443-3, RR490-3, and NN-3 Tested on Test-3 Ensemble.

Statistical Parameter	RR443-3	RR490-3	NN-3
RMS error ($mg.m^{-3}$)	2.03	1.63	0.730
rel. RMS error (%)	19.58	24.54	5.48
coeff. r^2 (%)	96.88	96.73	99.41

Figures Captions

Figure 1. NN architecture to model the inverse problem of ocean color. The $R_w(\lambda_i)$ are the five spectral marine reflectances and $F(\vec{R}, \mathcal{W})$ is the output of the network giving the estimated pigment concentration, C.

Figure 2. Scatter-plots of calculated versus desired pigment concentration. (a): Test of NN-1 with Test-1 data. (b): Test of NN-2 with Test-2 data.

Figure 3. Scatter-plots of calculated versus desired pigment concentration. (a): Test of NN-2 with Test-1 data. (b): Test of NN-1 with Test-2 data.

Figure 4. Scatter-plots of calculated versus measured pigment concentration. (a): Test of NN-1 on CalCOFI data. (b): Test of NN-2 on CalCOFI data.

Figure 5. Scatter-plots of calculated versus measured pigment concentration. (a): Test of RR443-1 on CalCOFI data. (b): Test of RR490-1 on CalCOFI data.

Figure 6. Relative RMS error obtained using NN-2, RR443-1 and RR490-1 on CalCOFI data.

Figure 7. Scatter-plot of calculated versus desired pigment concentration. Test of NN-3 on Test-3 data.

Figure 8. Scatter-plots of calculated versus desired pigment concentration. (a): Test of NN-3 on Test-1 data. (b): Test of NN-1 on Test-3 data.

Figure 9. Scatter-plot of calculated versus desired pigment concentration. (a): Test of RR443-3 on Test-3 data. (b): Test of RR490-3 on Test-3 data.

Figure 10. Relative RMS error obtained using NN-3, RR443-3 and RR490-3 on Test-3 data.

Figure 11. SeaWiFS-derived marine reflectance, R_w, at 412, 443, 490, 510, and 555 nm off the California coast on March 11, 1998. Negative reflectance values are displayed in yellow.

Figure 12. Phytoplankton pigment concentration deduced from the marine reflectances of Fig. 11 using the OC2-M algorithm and the NN-3 model. The difference between OC2-M and NN-3 pigment concentrations is also presented (lower left). Study areas are displayed in blue and green (upper right).

Figure 13. Phytoplankton pigment concentration derived by OC2 and NN-3 along the transect depicted in Fig. 12. Note the large pixel-to-pixel variability in the OC2 values, probably due to imperfect atmospheric correction.

Figure 14. Structure function, SF, as a function of sample distance, d, for OC2 and NN-3 in the rectangle area depicted in Fig. 12. At small distances, the NN-3 values are much smaller than the OC2 ones, indicating less sensitivity to atmospheric correction errors, as predicted theoretically.